Conceptual design and simulation of synthesis of 2-Methyltetrahydrofuran from furfural

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Summary

This project proposes an alternative to organic solvents by the production of less harmful, less toxic and renewable compounds. The conceptual design of the production process of the green solvent 2-MethylTethrahydrofuran (2-MeTHF) which is an aprotic ether solvent partially miscible in water is presented. 2-MeTHF has been used in organometallic and biphasic chemical processes because its interesting combination of properties provides opportunities for process simplification [1]. It is proposed as an alternative of 3 common solvents, such as Tethrahydrofuran (THF), Dichloromethane (DCM) and Toluene, which have applications in the pharmaceutical, plastic, among other industries [2]. In order to develop a more profitable productive process a simulation will be performed in Aspen HYSYS allowing to understand better the synergy among the different process variables. Also, to create a more sustainable process, an energy integration is included. Finally to evaluate the economic feasibility of the project, a cost analysis is carried out before and after optimization using process design tools with the support of Aspen HYSYS Economics. The result of this work was a design and simulation (case 1) of a process for the production of 2-MeTHF at high purity (~99%) and integrate energetically using HEN methodology (case 3) and reuse of utilities (case 2). Optimization can reduce total costs by 54% of the cost of manufacture.

1. Introduction

Solvents are substances that can dissolve gases, solids or liquids without the occurrence of any chemical reaction. They have a wide application in industry including purification, dispersion and synthesis processes. However, some of the most commonly used organic solvents are toxic, volatile, flammable, and harmful to the environment [3].

In order to decrease these impacts, green solvents are being developed, such as 2-MeTHF which is based on renewable materials with a low carbon footprint. This substance can be used as a solvent for most organometallic reactions replacing THF, DCM and toluene, which are petrochemical derivatives used in the manufacture of plastics, pharmaceutical, coating, magnetic tape, paint, adhesive, foam, metal clinic manufacture, among other industries. 2-MeTHF has a limited miscibility in water allowing an easy separation and recovery, reducing any waste in steam, eliminating the need of co-solvents (toluene) and reducing overall CO_2 emissions. Unlike THF which is completely water miscible, 2-MeTHF has higher reaction and extraction yields, and higher Gringnard reagent solubility. Also, 2-MeTHF has energy requirements similar to those of THF during the recovery process and distillation due to its low heat vaporization. Moreover, it has a lower peroxide formation, does not require a stabilizer, and it has a higher boiling point compared to THF reducing

overall reaction time [4]. 2-MeTHF can also be used as an efficient replacement for DCM in biphasic reactions like alkylation, amidation and nucleophilic substitution reactions [2].

2-MeTHF manufacture process uses only water as solvent and hydrogen obtained from natural gas. This solvent has a very low carbon footprint compared to other commonly used solvents, as shown in figure 1[4].

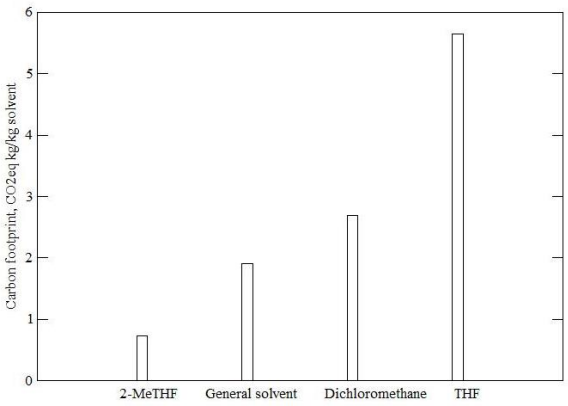

Figure 1. *Carbon footprint for selected solvents [4]*

The main material for the production of 2-MeTHF is furfural (FAL), which is produced from agricultural waste that contain pentosans, which are hydrolyzed to FAL and other by-products. FAL helps to convert abundant lignocellulose raw materials into ethanol and chemical co-products of greater value. The most common raw materials for FAL production include corn (main source), sugar cane bagasse, waste paper pulp, bamboo, kenaf, cereal husks, wheat and rice straws, nut shells, cottonseed and wood (hard and soft) [5].

The Strong shift towards the development of bio-based chemicals on account of volatile petrochemical prices and growing environmental concerns is expected to remain a key driver for the growth of global furfural market. A strong push for sustainable chemistry on a political and regulatory level across key regions is expected to play a critical role in furfural market development [6].
Furfural continues to grow as a result of strong demand for furfuryl alcohol to produce furan resins and increased furfuryl alcohol exports. In Figure 2, a pie chart of the world consumption of furfural in different countries in 2015 shows that China is the dominant player in the world furfural market with 75% of world consumption in a sample of 100% [7].

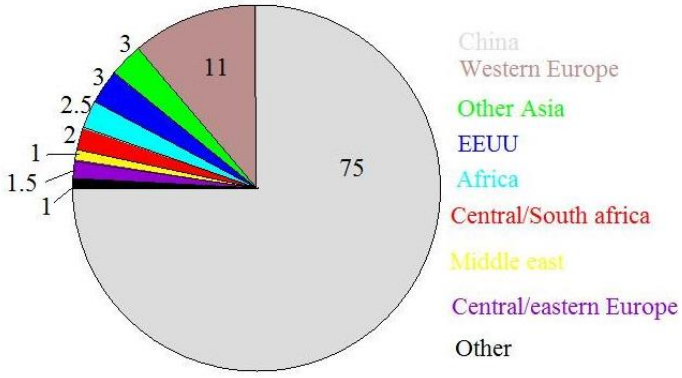

Figure 2. *World consumption of furfural – 2015 [7]*

Global exports of solvents from Colombia in 2016 were only around 56,000USD. The behavior of exports from Colombia during a period of 9 years, shows a decrease starting in 2008 with 156,000USD and culminating with 56,000USD in 2016 [8]. Colombian exports of solvents have two critical points, the first one is in 2011

where there is a significant fall attributed to two main indicators: the increase of the Colombian peso exchange rate and an increase in local production represented in the rise of the gross domestic product (GDP) in that same year, see the graphics in Annex 1. The second critical point occurred in 2016, being the lowest point in the last 9 years considered due to the large supply of solvents in the world with very competitive prices for the Colombian market.

On the other hand, the behavior of Colombian solvent imports has been increasing, with an 88.39% increase from 2008 to 2016 [8]. Imports show an exponential rise between 2011 and 2013 only with USA that might be due to the implementation of the free trade agreement (FTA) with USA, which is also related to the fall in exports in 2011.

This project seeks to assess these opportunities in the Colombian market with local products, replacing part of these import needs for solvents.

The aim of this project is to design, simulate and optimize the production process of 2-MeTHF in Colombia in order to gain knowledge of this novel solvent with a large number of potential applications, which could be a very interesting process to be developed in Colombia. Also, the use of this product will allow to reduce the use of hazardous solvents that affect negatively the environment, the economy and human health. A possible implementation of this project would allow to supply the import market for solvents and contribute to an increase in the GDP of the country.

There are few studies reporting the production of 2-Me-THF from FAL. Penn A Kem is a high-tech specialty chemical company with a product portfolio based on FAL and Furan made from renewable resources that supports a wide range of specialty applications. This company developed a successful production process for 2 MeTHF [9]. One of Penn A Kem's customers in the UK developed and implemented successfully the first industrial process using 2-MeTHF as a replacement for DCM. 2-MeTHF was superior to all other solvents as a DCM substitute according to data reported by this customer [10].

Another possible process for production of 2-MeTHF is presented by Irshad Ahmed et al [11]. This work created the productive process of 2-MeTHF from FAL, additional details are presented in Annex 2.

Although 2-MeTHF is a new solvent with a large potential use as a substitute for chlorinated solvents, more studies are required in order to understand, and possibly optimize its production process. 2-MeTHF can provide a broad solution to greener processes in a cost-efficient manner. This work will take into account the most relevant information of the works of Penn A Kem [4] and Irshad Ahmed [11] and use it to generate new proposals for the industrial production of 2-MeTHF.

2. Methodology

2.1. *Conceptual design*

The process have two main raw materials, hydrogen and FAL, both were investigate in order to know the physical and chemical properties, their market availability, consumption and production all over the world using Trademap tool [8]. For our process it is very important the procedure of the FAL because the aim of our project is based in green chemistry, that's why we sought suppliers of FAL that obtain this material from renewable source mentioned before. Properties, suppliers and extra information about FAL are specified in Annex 3. Other inputs of the process are the catalyst, copper based and nickel based, both required in the reactions, and also their physical and chemical properties are described in Annex 4.

The utilities of the process are other process inputs not considered as raw materials, in this case it is necessary a hot stream and a cold stream to condition the streams of the process.

The process specifications and analysis of the reactions was carried out to determine the products and by-products[10], also the consumptions[7], [12], market[8], uses and physical and chemical properties[1] were

investigated. Once all this information was obtained, a process diagram of inputs and outputs (PDIO) was implemented to have a better understanding. Then, the mass balance was performed and implemented in a process block diagram (PBD) identifying the composition of the currents. Moreover, the economic potential was calculated. The equipment specification required for the design and simulation of the process was done using heuristic rules [13]. The piping and instrumentation diagram (P&ID) was built, with flows, control loops, capacity and industrial utilities. All the diagrams were made using the online program Draw.io following ISO 10628 standards [14].

2.2. *Simulation in Aspen HYSYS (case 1)*

The process was simulated in Aspen HYSYS V8.8 [15], the components list according to the program nomenclature were: Furfural, Hydrogen, Water, Furfuryl alcohol (Furfurol), 2-Methylfuran (2-M-furan), Tetrahydrofurfuryl alcohol (THyFurfurol) and 2-Methyltetrahydrofuran (2-M-4HyFuran). The thermodynamic package used was Non Random Two-Liquid (NRTL), which calculates the activity coefficients in the liquid phase of the phases present in the process. This model is used for systems that have a wide range of boiling point between the components. At the same time the Lee-Kesler-Plocker equation is used because it is the most accurate general method for non-polar substances and mixtures [16].

A validation of the NRTL model was made through a comparison with experimental data [17] using case studies in Aspen HYSYS, as shown in figure 3.

It is important to highlight one of the difficulties with the default binary interaction parameters of NRTL for Aspen HYSYS V8.8, this model showed deviations to replicate the behavior of the liquid phase respect to the experimental data, however the vapor phase was reproduced well, so the model was we decided keep the model because the principal part of our process happen in vapor phase.

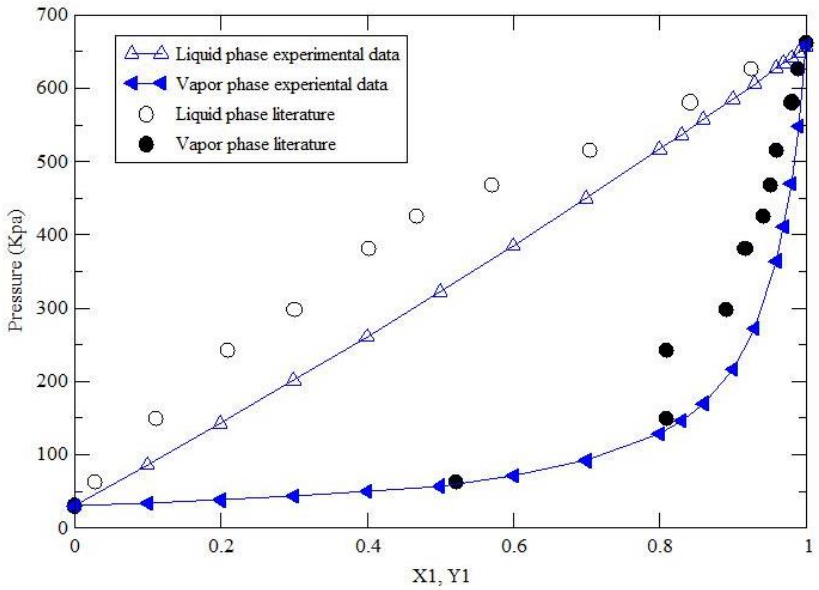

Figure 3*. Vapor-liquid equilibrium of 2-methylfuran (1) and furfuryl alcohol at 408.2 K*

Binary coefficients used to adjust correctly the behavior of the process as shown in table 1. All the values of the components mentioned before on the component list were completed using UNIFAC, a system for the prediction of binary coefficients of calculation of activity in non-ideal mixtures, for vapor-liquid-liquid equilibrium (VLLE) and the interaction parameters of 2-MF and water were calculated considering the components as inmiscible [18].

Table 1. *NRTL binary coefficients for the component involved in Aspen Hysys.*

	Furfural	**H_2**	**Furfurol**	**2-M-Furan**	**H_2O**	**2-MeTHF**
Furfural	-	11,56	87,21	1264,13	1309,69	775,19
H_2	1307,63	-	1689,66	692,49	8,02	540,77
Furfurol	200,84	11,56	-	-	1826,43	-
2-M-Furan	-153,11	11,60	-	-	605,00	-
H_2O	219,89	-6,51	291,86	8114,73	-	414,46
2-MeTHF	-15,40	11,60	-	-	3070,00	-

The kinetic reactions of the productive process were taken from Tseng et al. [19], equation 1 is the hydrogenation of FAL to Furfurol, equation 2 is the hydrogenation of Furfurol to make 2-M-furan and Water, those two reactions in series take place in the first reactor. The second reactor has two parallel reactions, equation 3 describes the hydrogenation of 2-M-furan to produce 2-MeTHF and equation 4 is another possible result of the hydrogenation reaction which produces Tetrahydrofurfuryl alcohol as byproduct.

$$Furfural + H_2 \rightarrow Furfurol \ (1)$$

$$Furfurol + 2H_2 \rightarrow \ 2 - M - Furan + H_2O \ (2)$$

$$2 - M - Furan + 2H_2 \rightarrow 2 - M - 4HyFuran \ (3)$$

$$2 - M - Furan + 2H_2 \rightarrow Tetrahydrofurfuryl\ alcohol \ (4)$$

The influence of temperature on the rate of chemical reactions can be described by the Arrhenius equation. According to this, a rate constant k is the product of a pre-exponential ("frequency") factor A and an exponential term equation 5 where R is the gas constant and E is the activation energy [20].

$$k = A * exp\left(-\frac{E}{RT}\right) * T^b; T\ in\ Kelvin \ (5)$$

Although the Equation 2 is theoretically reversible, the equilibrium constant is shifted to the products which allows a conversion greater than 99% at standard operating conditions, therefore many of the kinetic models published in the literature approximate the reaction as irreversible[21]. Several authors [22]have studied the hydrogenation of furfural and reported kinetic data and/or kinetic models for the reaction. Several types of catalysts have been studied for this reaction, including copper chromite [23], copper/sodium silicate [24]and platinum catalysts [21]. Copper chromite is the most widely used catalyst in the industry [25] and offers good yield and high selectivity to furfurol with 2-M-Furan and water being the only significant by product. Thus, in this work the kinetics reported by Borts et al. using a copper chromite catalyst are employed equation 6 [19].

$$r_{Furfurol} = 3{,}14x10^{16} * exp^{\frac{-10740}{T}} * C_{Furfural} * {C_{H_2}}^2 \ (6)$$

Where the concentration of reactants $C_{Furfural}$ and C_{H2_2} are in mol/L and the temperature T is in Kelvin. Borts et al. do not provide data or a kinetic model for the rate of the 2-M-Furan reaction. However, information about the production of 2-methylfuran at 99% conversion of furfural and at different temperatures is provided by Zeitch[25]. The data reported by Zeitch was used to regress parameters of a kinetic rate expression for equation 2 and the result is show in equation 7 [19]. For equation 3 and 4 no reaction rates are reported in the open literature, thus it was decided to model them as a conversion process.

$$r_{2-M-Furan} = 1{,}41x10^{20} * exp^{\frac{-19000}{T}} * C_{Furfurol} * C_{H_2} \ (7)$$

Using these specifications a base case was implemented in Aspen HYSYS and it was used as the initial values for the optimization.

2.3. *Energy optimization*

The first proposal for improving the process was to include a recycle of utilities, water and thermal oil. A design was made to include reuse and take advantage of the remaining energy.

Then a process integration method was proposed to reduce costs. The method was based on the pinch method for the design of an energy exchange network (HEN) that seeks maximum use of energy to generate monetary savings through the process heat exchanger connection. The integration can reduce the consumption of diverse sources of energy.

For the identification of energy recovery systems, it is necessary to follow these steps [26]:

1. Check the general process diagram with the heat exchangers.
2. Convert the heat exchangers into heaters and coolers.
3. Analyze the behavior (linear/non-linear) of the heaters/coolers temperature (T) vs enthalpy (ΔH) and in case it is not linear divide the stream in linear sectors.
4. Tabulate streams: the streams to be heated are referred as cold streams and the flows for cooling are recognized as hot streams. Information on the inlet and outlet temperatures of the heat exchanger, the ΔH and the calorific capacity (Cp) are also tabulated.

The grand composite curve (GCC) reveals opportunities for replacing utilities and improve energy efficiency, to construct this curve is necessary to execute the following calculations:

1. Calculate the shifted temperature (T *) of the process stream.
2. Define the temperature ranges.
3. Calculate the thermal balances of the intervals (H).
4. Assume the heating service as zero and perform cascade calculations (heat accumulated). The temperature intervale where the accumulated heat is zero is defined as the pinch point.

Finally, with the calculated data and the matching of streams to integrate energy utilization, the integrated process was simulated in Aspen HYSYS. The objective was to maximize the use of cheaper utilities and minimize the use of the more expensive utilities. Also the E-factor was calculated for the three cases, this allows to see which of them is the most ecological.

2.4. *Cost calculation*

The calculation cost of the plant was based in module costing technique by Turton et al[27]. This technique relates all costs to the purchased cost of equipment evaluated for some base conditions. Deviations from these base conditions are handled by using factors that depend on the specific equipment type, system pressure and materials of construction [27].

Variables like bare module cost (C_{BM}), total module cost (C_{TM}), grass roots cost (C_{GR}), operating labor cost (C_{OL}), utility total cost ($C_{UT\ TOTAL}$), raw materials total cost ($C_{RM\ TOTAL}$), land cost (C_L), cost of manufacture without depreciation (C_{OMd}) and the revenue were calculated for the economic analysis. Also Chemical Engineering Plant Cost Index (CEPCI) was adopted to adjust the effects of inflation on equipment costs from 2001 to 2015. The complete financial analysis of the process was used to assess the economic viability of the project. This analysis was done for the process before and after optimized case and compared in order to determine the effect of optimization.

3. Results and analysis

3.1. *Conceptual design*

According to the reactions of the productive process of 2-MeTHF, the inputs and outputs diagram was built, where the raw material, products and byproducts are specified, see figure 4.

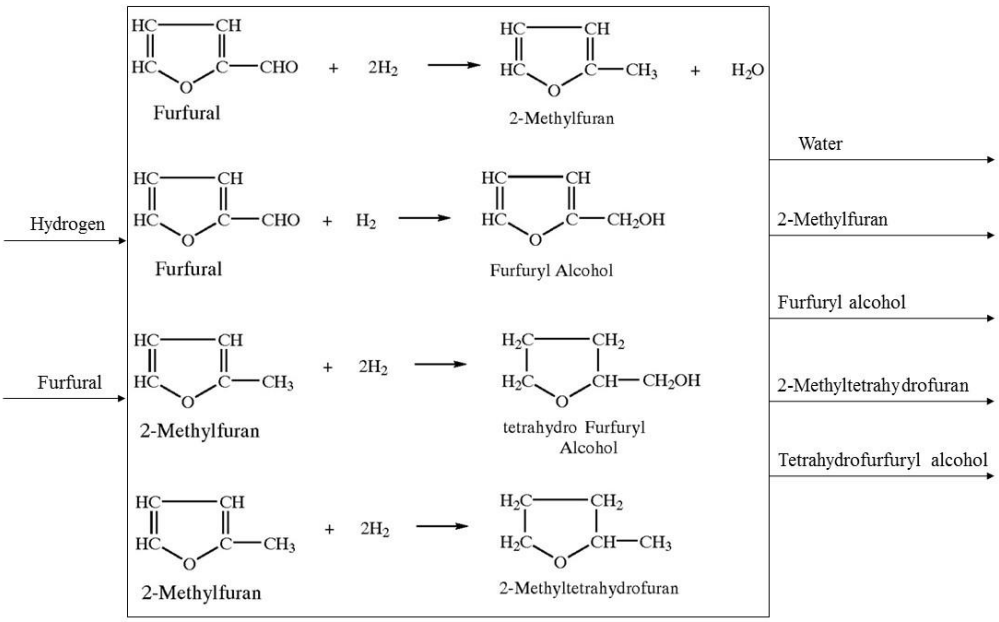

Figure 4. *Process diagram of inputs and outputs*

The process starts in the vaporizer, where FAL is vaporized and mixed with hot hydrogen gas, then the mixture goes to a plug flow reactor (a packed fixed bed) which contains the reduced copper based catalyst. There the exothermic catalytic hydrogenation of FAL takes place. The vapor phase hydrogenation was run at 180°C. The products pass through a heat exchanger which allows to turn the vapor mixture into a liquid-liquid equilibrium, containing in the organic phase, 2-M-Furan, and an aqueous phase containing furfurol and water these two phases can be separated in a liquid-liquid separator tank [11].

The 2-M-Furan free of furfurol can be vaporized and mixed with hot hydrogen gas and delivered into a second plug flow reactor where the temperature is maintained at 180°C. This second reactor contains a reduced nickel based catalyst. The vapor phase mixture produced in the second reactor is composed of 2-MeTHF and the byproduct Tetrahydrofurfuryl Alcohol, which is condensated and it is also separated in a liquid-liquid separator tank. The molar ratio of the hydrogen to furfural in the first reactor and the hydrogen to 2-M-Furan in the second reactor is 2:1 [11]. In this work pentane and pentanol produced in the second reactor are taken as impurities and ignored for the process calculations.

Knowing the process and considered a capacity to produce 70.000 Ton/year thinking about supply the local demand of 2-MeTHF previously discussed, a mass balance and economic potential (around $14,977 million USD) were made based on the information in the patent investigation [11], details of the calculations is included in Annex 5. Also, the P&ID were made; see the Figures in Annex 6 and 7 respectively.

3.2. *Simulation in Aspen HYSYS*

Figure 5 shows the Aspen HYSYS simulation environment and the naming conventions used for process streams and unit operations. This section highlights the changes or considerations different from the design section and this is because at each stage of the project the production process was refined to make it as realistic as possible.

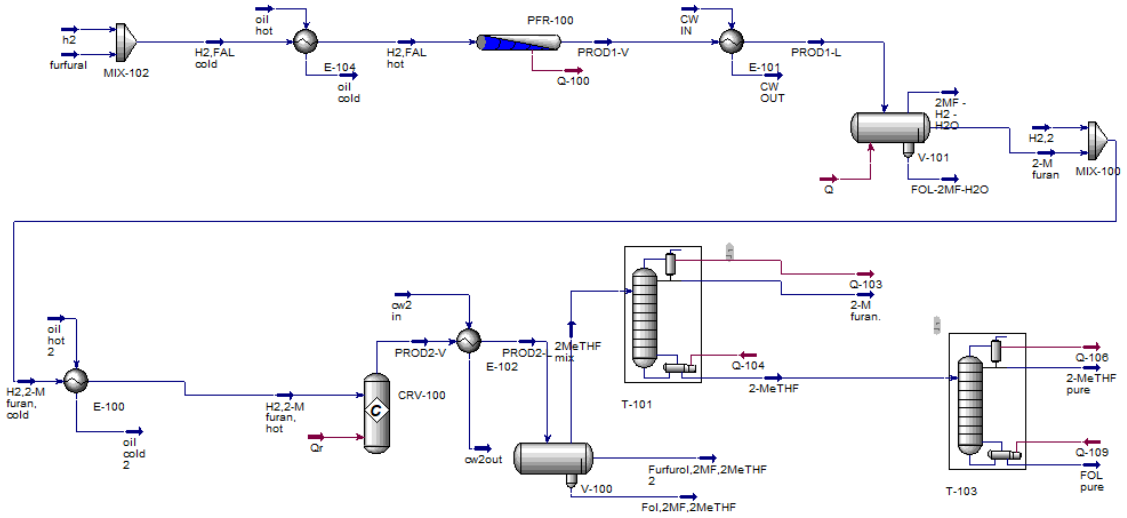

Figure 5. *Aspen HYSYS simulation flowsheet for the production of 2-Methyltetrahydrofuran*

First the furfural liquid and gaseous hydrogen were mixed and then heated in a shell and tube heat exchanger with thermal oil service (MT-IG-2 at 390°C).Then, the mixture, in vapor phase (H2 and FAL at 340ºC) goes into a plug flow reactor (PFR). High temperature is required in order to produce a large selectivity of the compound of interest, 2-M-Furan and avoiding formation of furfurol. This first reactor has two reactions that were modeled as heterogeneous catalytic because the reaction rate equation is not elementary. In addition, the reactor is cooled down using water at 25°C since the reactions are exothermic and the operating conditions were isobaric and isothermal at 1 atm and 340°C. This reactor has a conversion of 96%. The process continues with cooling the mixture with cold water at 25°C in a tube and shell heat exchanger for enter to a liquid-liquid (L-L) separation which divides the mixture into three phases, two liquid, 2-M-Furan/furfurol and water, the other phase is steam with 2-M-Furan, hydrogen and water. Streams with water and steam come out of the process and the one with 2-M-Furan and furfurol continues through the process. The latter is heated up to enter in the second reactor, which is modeled as a conversion reactor with a conversion of 89% based on experimental data due to the lack of information on the kinetics. The conditions of operation of this equipment were 1atm and 300°C. Like the first reactor, this reactor is conditioned with chilled water at 25°C. The conversion of the reactor in the simulation differs with the experimental data, obtaining a conversion reaction of 68% because although reactor conversion is set at 89%, due to phase changes some of the reactant is condensed and does not react.

Then the outlet stream from the second reactor was cooled down with cold water at 25°C in a tube and shell heat exchanger to continue with a liquid-liquid separation that separates most of 2-MeTHF, which continues the process and goes to the distillations towers to finish the process of separation.

3.2.1. *Technical specifications equipment*

All the heat exchangers used are shell and tube and the industrial utilities are thermal oil (MT-IG-2) [28], with a boiling temperature of 435.6°C, for heating and cold water at 25°C for cooling. The utility goes into the shell while the main streams go into the tubes, this is because the more viscous fluid must travel through the shell to have a lower pressure drop. The heat exchanger has one pass through the shell and two passes through the tubes, this is because all the tubes form a U inside the shell [29]. All the heat exchangers present the same configuration; the utilities go into the shell, two steps through the tube and one through the shell.

For both liquid-liquid (L-L) separations before the reactors a 3-phase separator was used, which divides the mixture in a light and a heavy phase. This equipment can separate a vapor, a liquid and an aqueous phase. The effectiveness of this separation depends directly on the inlet temperature and this is the reason why a heat exchanger is placed before, because the lower the temperature the higher the separation. This type of separator

was chosen because it can work at atmospheric pressure and it has lower capital and operating costs than a countercurrent separation tower.

Finally, with a vapor phase rich in 2-MeTHF a distillation tower was used to purify this substance. First, a shortcut tower was built to provide information about the feeding tray and total number of trays for a rigorous distillation tower. The final product was obtained with purity of 94% of 2MeTHF. To maximize this purity a second tower was built to separate the little amount of furfurol remaining in this stream, the procedure of a shortcut and a rigorous tower was developed once again in order to obtain the highest purity (~99%) of our interest compound. Finally a second tower was used to get 99% purity of 2-MeTHF.

3.3. *Energy optimization*

3.3.1. *Recirculation of utilities (Case 2)*

To optimize the process and reduce costs, it was proposed to recirculate the utilities of the process. Initially the utility implemented to heat was thermal oil, because it is thermally the most suitable compound to work at high temperatures, however it is not necessarily the most economically efficient utility. So it was proposed to replace it by a natural gas burner, implementing a fired heater with the ability to work at high temperatures, satisfying the heat needed of the exchangers and in turn obtaining a significant cost reduction. This equipment is dynamic and works with inputs of air and fuel (methane), and an efficiency of 45% and oxygen excess of 10%, also the outlet flue gas is reused for heating the third heat exchanger of the process replacing input of thermal oil [30].

On the other hand, the industrial utility for cooling was water, and the whole thermodynamic cycle was considered. Thus, a cooler was considered (representing a cooling tower) and a pump to regulate the pressure changes in the loop, the same system was implemented for both cold heat exchangers in the process. The flowsheet of the process simulation implemented on Aspen HYSYS is shown in figure 6. For details go to Annex 10.

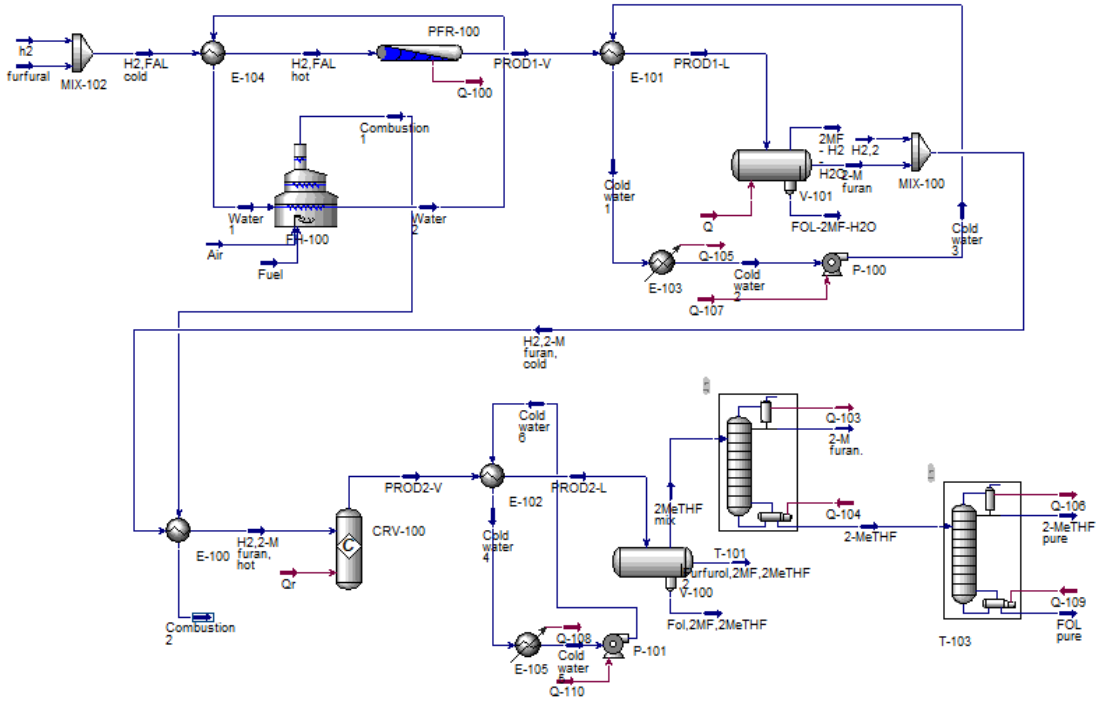

Figure 6*. Simulation of recirculation of utilities on Aspen HYSYS*

3.3.2. *HEN methodology (Case 3)*

The process requires four tube and shell heat exchangers, two of them used cold water (E-101 and E-102) while the other two (E-100 and E-103) used thermal oil in order to heat cold streams.

In this case, two of the heat exchangers presented a non-linear behavior in the T vs ΔH plot, so it was necessary to divide these flows according to the behavior of the heat exchangers. Also, a minimum temperature difference (ΔTmin) of 10°C was used [26].

For the integration of the streams, the grid diagram is constructed based on the pinch methodology, where hot streams 2 (PROD1-V) and 4 (PROD2-V) entering the pinch and the cold streams 3 (H2, 2-Mfuran, cold) and 1 (H2, FAL cold) leaving the pinch are identified visually. In this same diagram it is evident that all the currents are above the pinch and only heating utility is required in the process. See Figure 7 to details of the grid diagram.

For matching the streams for the integration, it is proposed to match stream 3 (the smallest heat requirement of the cold streams) with both hot streams, however this only heats this stream up to 272.17°C and additional industrial utility is required to complete the heating process up to 300°C, to achive the temperature required, the stream was heated to 300°C with the help of the fired heater using 10% of Oxigen and with an efficiency of 70%

The cold stream 1 was not matched due to the high requirements and to have a lower number of heat exchangers no splitting of the streams was required.

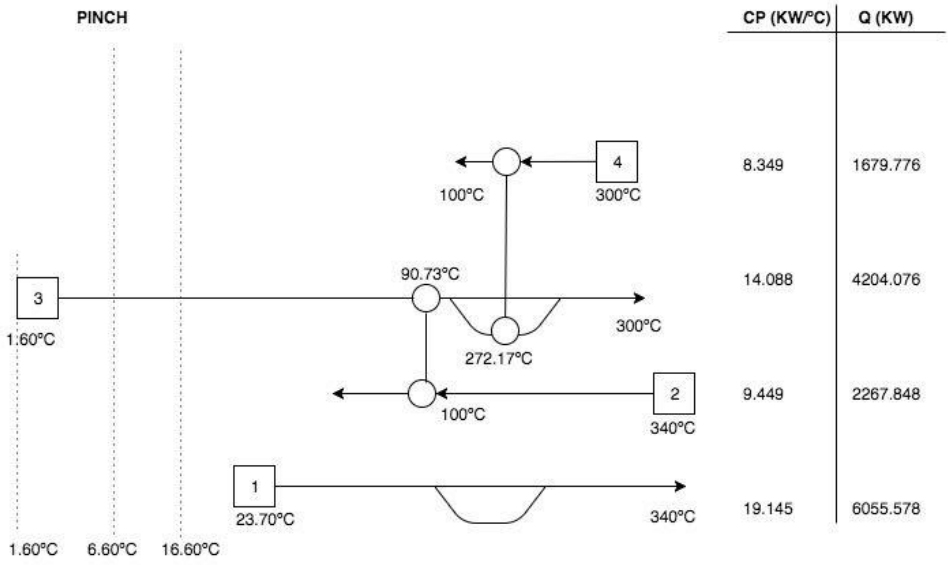

Figure 7. *Grid diagram for integration HEN methodology*

Having the integration network defined, the integrated process is simulated in Aspen HYSYS and the system costs are calculated before and after the optimization, based on the requirement of utilities for heating and cooling. See calculations details in Annex 8. Figure 8 show the simulation of the optimization of the process.

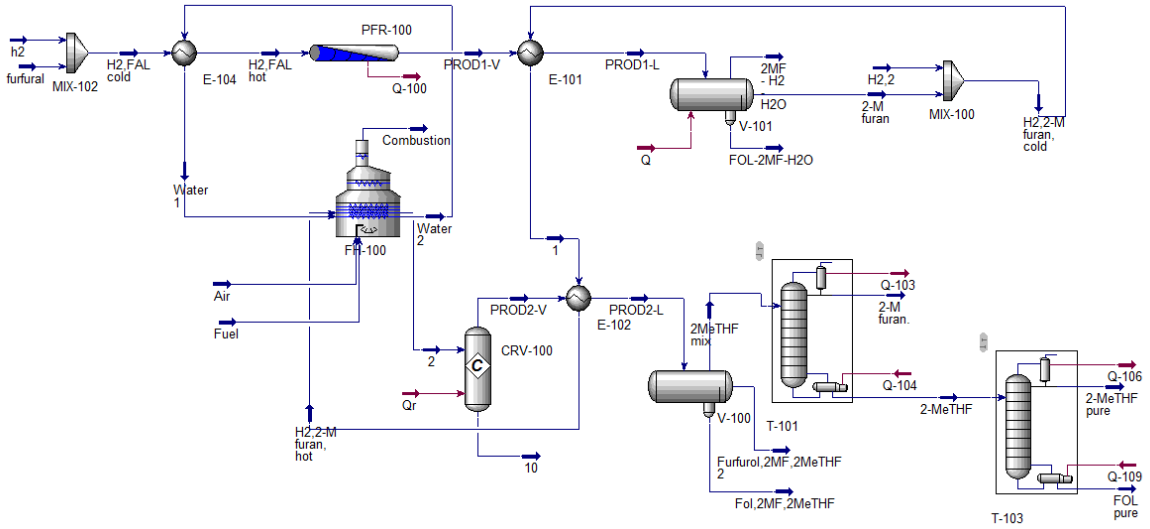

Figure 8. *Simulation of HEN methodology process*

The E-factor was calculated for the tree cases, case 1 present an E-factor of 144.28, case 2 of 2.33 and case 3 of 1.99. Case 1 has the highest E-factor because it does not have recirculation of utilities, therefore it has a lot of process output streams. Case 2 is larger than case 3 because it requires more methane in the process that will later be released to the atmosphere, leaving case 3 being the most environmentally friendly.

3.4. *Cost calculation*

The analysis of the costs is based on three scenarios; case 1 is the base simulation without any economic savings attempted.. In scenario 2 are analyzed the economic impacts caused by the recirculation of utilities and the change of substances for heating streams, although it was assumed that the cold water its being recirculate and need to be changed every period due to the accumulation of oxidizing compounds that over time deteriorate equipment and pipes that can end in leaks [31]. The case 3 part from the recycle of the utilities and integrates the flows according to the HEN methodology. The economic impact is measure compared with the based case 1. The costs are divided and analyze separately by fixed capital investment, utilities cost and labor for each case in order to create a cash flow. Annex 9 show details of cost calculations.

3.4.1. Fixed capital investment

The equipment was considered made of stainless steel (SS) to prevent the corrosion and to ensure durability of the plant. Figure 9 show bare module cost of the process equipment (that change) for the tree cases, where the reactor PFR was the equipment with the highest cost for all the cases. The case 1 present a constant cost in their exchangers and the lowest cost in the separators, reactors and towers compared with the others cases. The case 2 have the biggest number of equipment and their coolers have a higher cost than the exchangers, because the conditions of the process. In cases 2 and 3 the PFR cost rises due to energy integration before and after this, demanding a higher contact area.

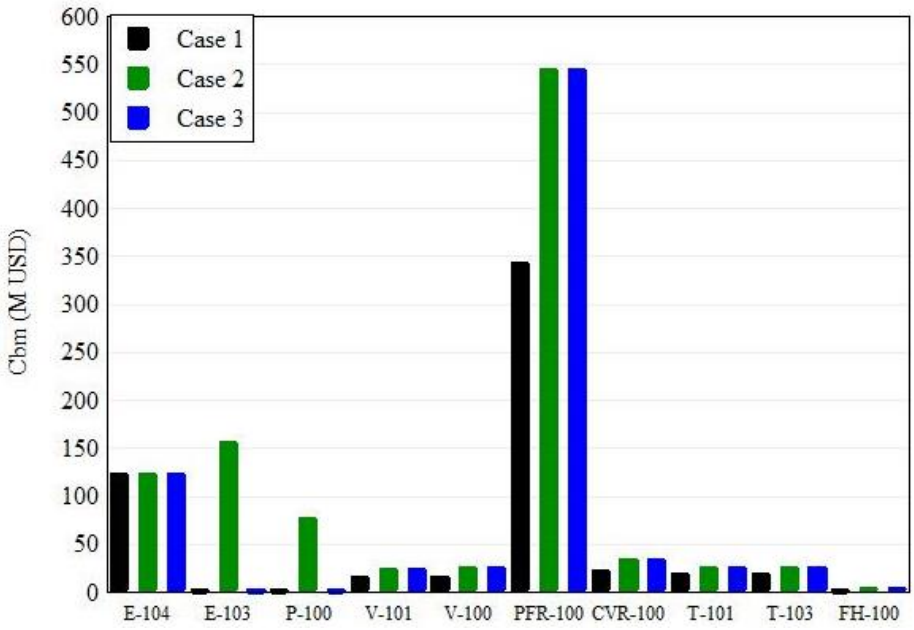

Figure 9. *Bare module cost of the process equipment for the tree cases*

The result of the equipment C_{BM} was used to calculate the grassroots cost (C_{GR}), which consider the cost of site development. Leaving the case 1 with the cheapest C_{GR} due to the reduce number of equipment employed and their conditions, with a cost of 1,646M USD. Follow by this, case 2 and 3 have a Cgr of 2,940M US and 1,864M US, respectively.

3.4.2. Utilities

According to the consumption of the utilities in the different cases, for one year of production, 279 days, shown in table 2, it is seen that the consumption of the hot utility decreases in case 2 and case 3 with respect to the case 1, due to the change configuration in the process. The decrease in consumption of the water is mainly because in Case 1 this utility is not being reused, whereas the electricity consumption in case 2 is the highest compared to the other, because it has additional energy requirements of the pump used for reuse of utilities. In conclusion the case 3 demands the least utilities consumption per year.

Table 2. *Consumption/year of utilities in the different cases in thousands of dollars*

Consumption/year of utilities			
	Case 1	**Case 2**	**Case 3**
Oil consumption (m3/year)	4747	-	-
Methane consumption (m3/year)	-	19	13
Water consumption (m3/year)	856	2235	1421
Electricity consumption (kWyear)	38,261,391	38,262,562	32,962,940

Analyzing the costs of the utilities, shown in table 3. The electricity is the cheapest utility (0.18$/kWh) but has the highest consumption in the process. Methane which cost 3.96$/m3 was change to thermal oil and performing a recirculation of the other utilities, costs can reduce by up to 71%, but comparing the energy integration (case 3) with recirculation (case 2) only 14% in terms of cost reduction. The most expensive scenario is Case 1 due to the high cost of thermal oil (3,000$/m3) and the constant flow of water which cost 1.2$/m3. Case 2 and 3 have similar costs differing only in 5% being case 3 the cheapest.

Table 3. *Cost of utilities/year for the different cases in thousands of dollars*

Cost of utilities/year in the different cases			
	Case 1	**Case 2**	**Case 3**
Oil ($/year)	$14,239,591	-	-
Methane ($/year)	-	$73.34	$52.97
Water ($/year)	$1,029.72	$2,691	$1,710.84
elect ($/year)	$7,040,671	$7,040,887	$6,065,677
Cut($/year)	$21,281,292	$7,043,652	$6,067,441

3.4.3. Labor costs

The labor costs are considered to be the same for the different scenarios, due to the number of operators is a global number for the productive process, and the number of the main unit operations was not increased in the different scenarios. The available men hours were stipulated considering the 17 holidays in average that has a year, the 52 Sundays and 17 days less by work of short shifts on Saturday, all this in order not to incur extras and to decrease the cost of operation. On the other hand, 13 workers were considered per shift, which represents a total of 19 workers in the plant, since the plant operates 3 shifts a day and it is considered that the 7 main equipment's operates with 2 people per shift. The annual labor cost in dollars calculated based on the minimum wage in Colombia of $278.80/month, which concludes that the labor cost per year is worth Col=$130,477.53USD.

Figure 10 shows the most influential variable in the calculation of the Comd is Cut. For case 1, the Comd is significantly higher, which confirms the less profitable case. For case 2 is shown a saving with respect to case 1 however case 3 is the one of greater saving. In addition, the revenue is constant because all three cases assume the same annual production and conversion of the process. In order to demonstrate information mentioned before, a cumulative cash flow is used to evaluate the behavior of the three cases over time.

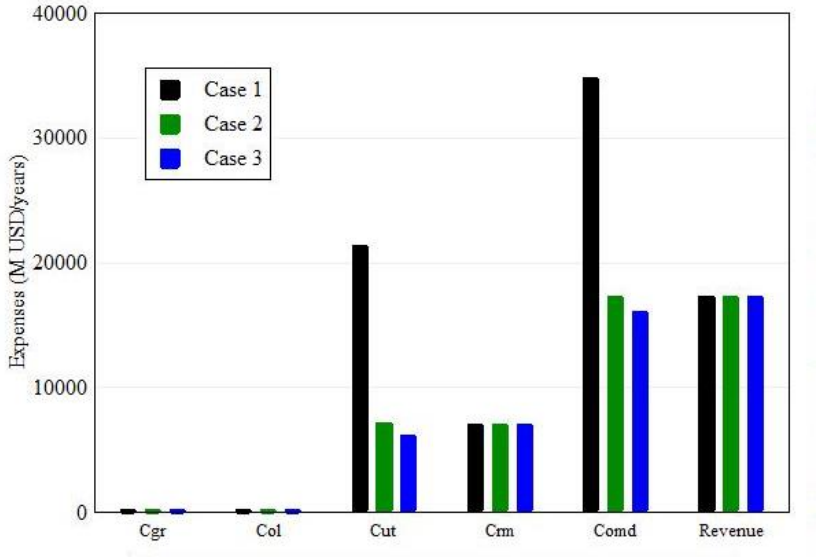

Figure 10*. Principal expenses for the cash flow calculations of the tree cases*

3.4.4. Cash flow

The cash flow was built with the past numerals for the tree cases. For calculations, it is considered a cost land of $152,839.24USD, a working capital (WC) of 20% of Cgr that was taken as the fixed capital investment (FCI), taxation rate (t) of 70% and payback period (PBP) of 3.85years.

aking a price for 2-MeTHF sale ($264,511USD/Ton) [2] to estimate the internal rate of return (IRR) of the process for the case 1, it was found out that the process was not profitable due to the revenue per year is lower than the variable cost. To make case 1 profitable with an IRR of 7% it is needed to increase the price of 2-MeTHF in 200% ($534,129.5USD/Ton). Case 2 present an IRR of 7% having incomes in the year 6. In the case 3 the IRR is 1087% which means that in the third year (first year of operation) will have incomes, this kind of profitability is unreal, the price of 2-MeTHF could be $246,035USD/Ton to have a IRR of 7% with incomes in the year 6. According to the information mentioned before the figure 11 show different 2-MeTHF's prices for an IRR of 7% in the process.

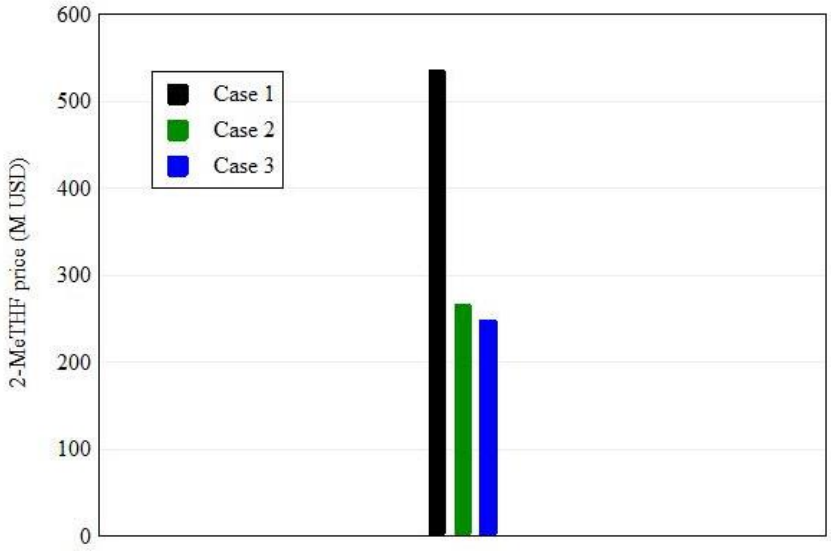

Figure 11. *Price of 2-MeTHF to IRR of 7% for the tree cases*

4. Conclusions

This project represent the different transformations of furfural from renewable sources which take place in the production of a green solvent (2-MeTHF) to replace traditional solvents of the industry and to generate a lower impact to the environment from the production to its final disposal. In order to assess the feasibility of the process, a plant for the production of 2-MeTHF has been designed, simulated and optimized.

The design of the base case was developed with bibliographical reviews and theoretical considerations going through a group of unitary process and chemical reactions. Thanks to the simulation it recreates and verifies the construction of the plant of 2-MeTHF, taking the process to more real conditions. Also involves an economical factor which revels the viability of this plant if it wants to be carried out.

Starting from the simulated case, there was an opportunity to optimize the process through the recirculation of utilities and energy integration. According on the results of the economic evaluation for the 2-MeTHF process, base on to case 1, it was found that case 2 decreases cost of manufacture from $34,696M USD to $17,181M USD and case 3 decreases cost of manufacture to $15,981M USD. Expecting to have an IRR of 7% in the project with incomes in the year 6, the price of 2-MeTHF should be in case 1 $534TUSD/Ton, in case 2 $264TUSD/Ton and in case 3 $246TUSD/Ton.

In the case 3, the utility expenses were significantly reduced and the cost of the equipment was reduced. With the changes that were made, according to the IRR values calculated, the optimized case 3 design was determined to be an economically feasible project. Lastly it is important to note that most of the expenses in this process

are associated with the cooling and heating equipment and with the utilities required for them. Therefore, the heat integration of the process helps to significantly reduce many of the expenses in the process. Also it can be concluded that case 3 is the most environment friendly, because it presented the smallest E-factor of 1.99. In conclusion, this Project is the compilation of the knowledge acquired during the course of engineering processes that allow to apply what has been learned to provide solutions to improve the life of society

5. Table of Annex or Appendices

Table 5 shows a link to additional information about the project. Also aspen HYSYS documents are presented in annex 11, 12 and 13.

Table 5. *Additional documents included in the project*

Name	Development (self/others)	Type of document	Google drive link (https://goo.gl/)
Annex 1	Self	Doc	https://goo.gl/koTg6w
Annex 2	Self	Doc	https://goo.gl/K9a7HG
Annex 3	Self	Doc	https://goo.gl/4bRfU2
Annex 4	Self	Doc	https://goo.gl/KLgQb4
Annex 5	Self	Xml	https://goo.gl/qn7uQe
Annex 6	Self	png	https://goo.gl/ziE4q4
Annex 7	Self	png	https://goo.gl/DfLSPx
Annex 8	Self	Xml	https://goo.gl/UJYVRZ
Annex 9	Self	Xml	https://goo.gl/hbtUwh
Annex 10	Self	Xml	https://goo.gl/eeCaJr
Annex 11	Self	Xml	https://goo.gl/UCtt6a
Annex 12	Self	Xml	https://goo.gl/EZGB2N
Annex 13	Self	Xml	https://goo.gl/cBfRua

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